

Fig. 1

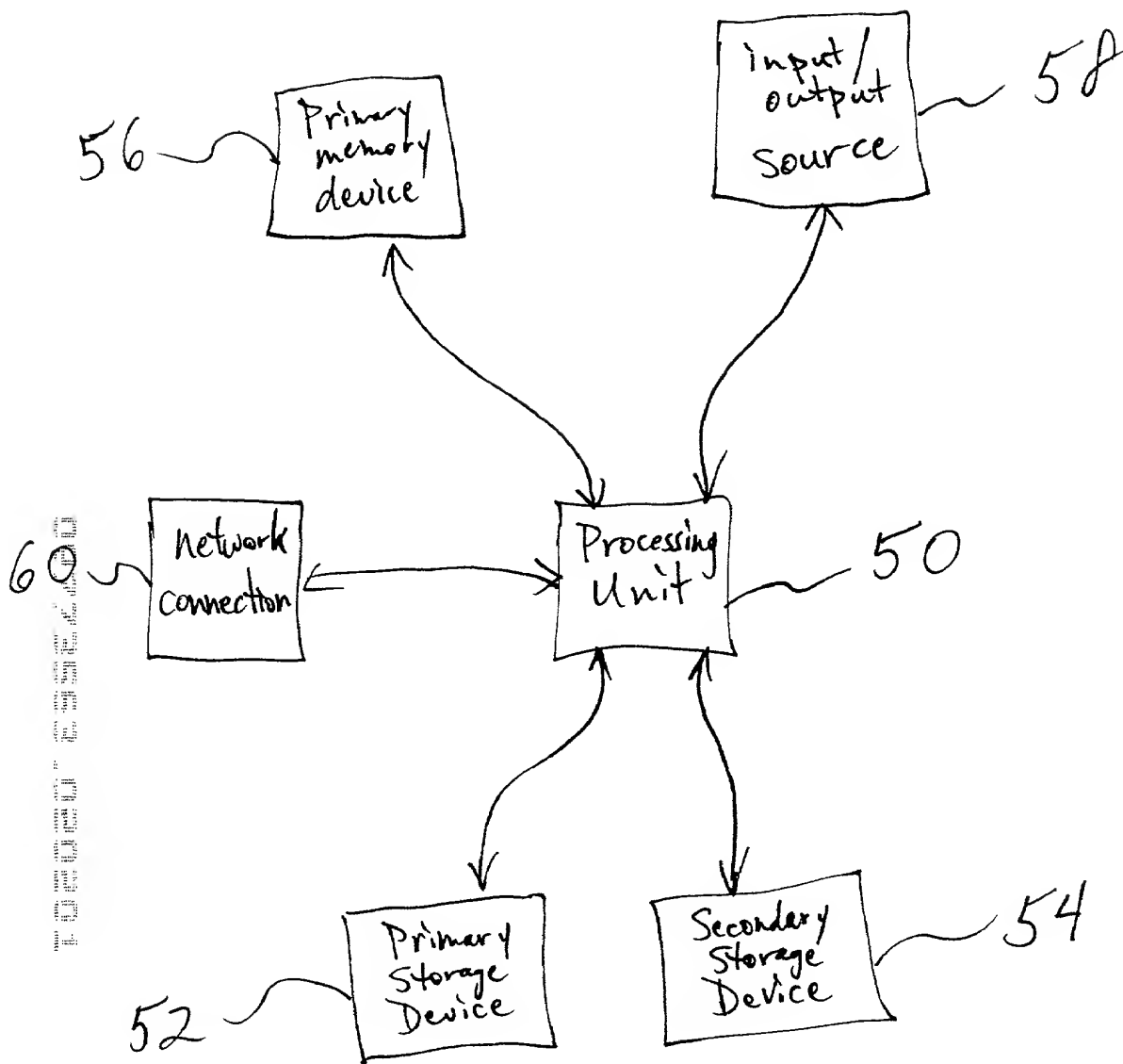


Fig. 2

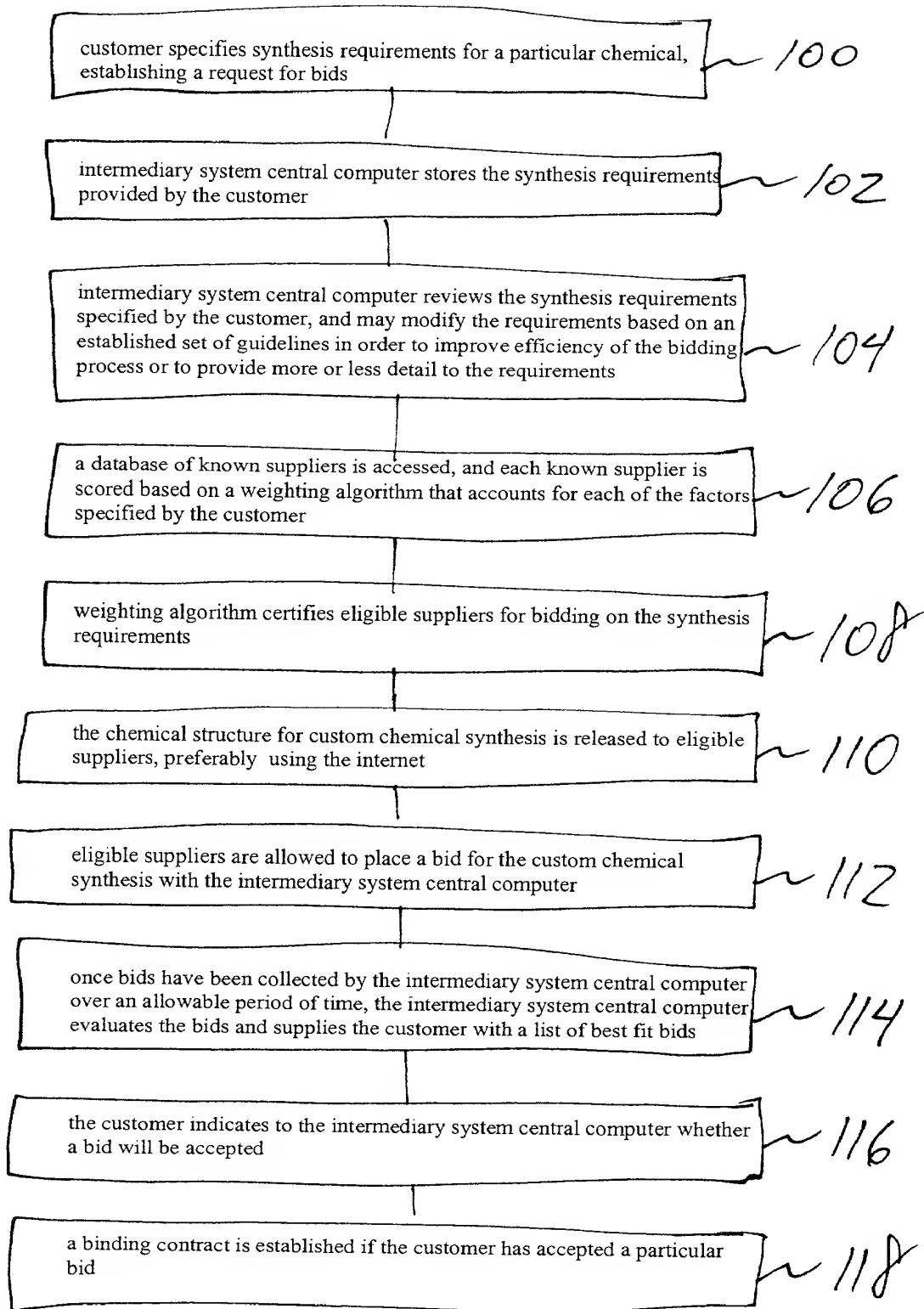


Fig. 3

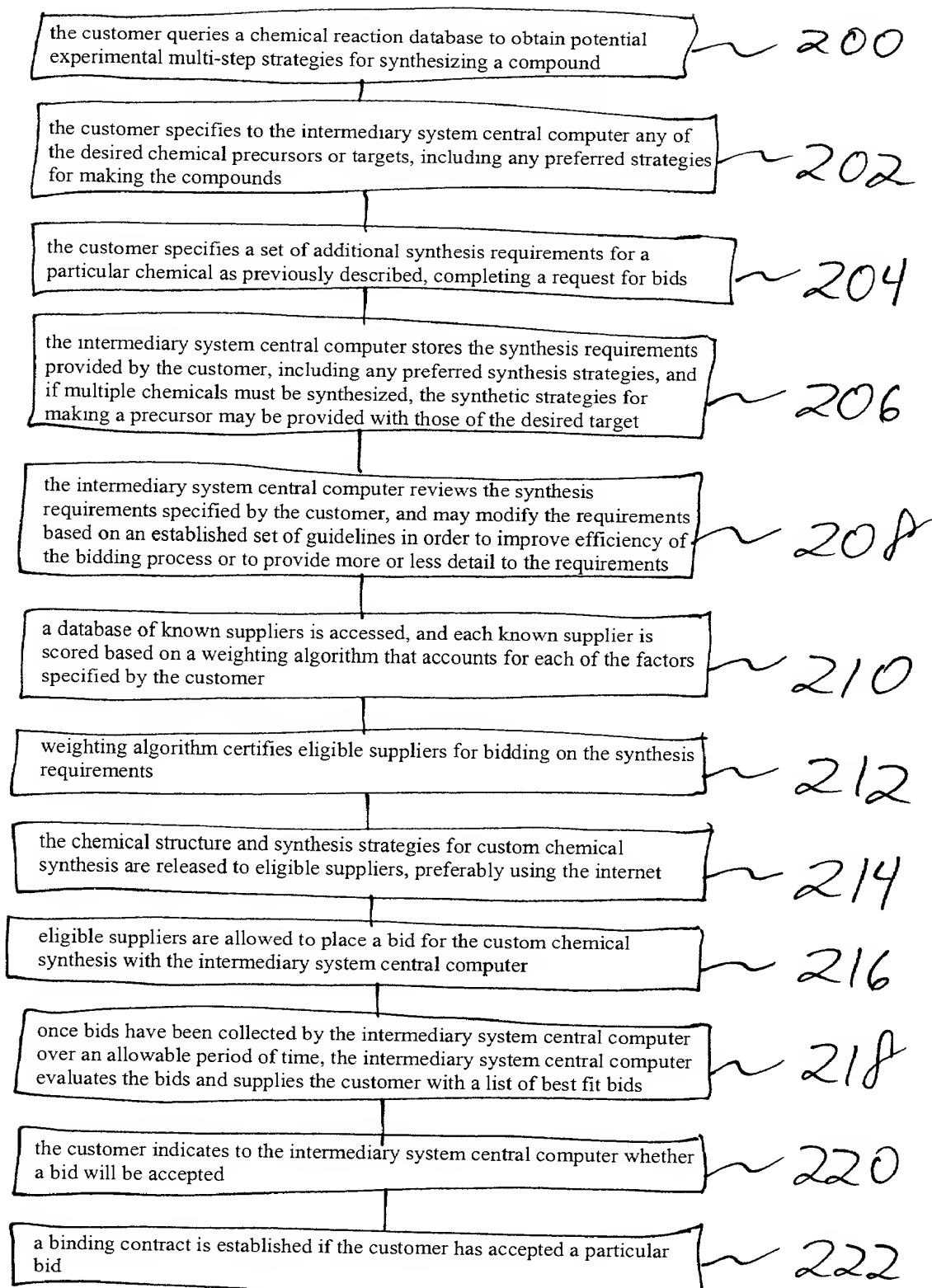


Fig. 4

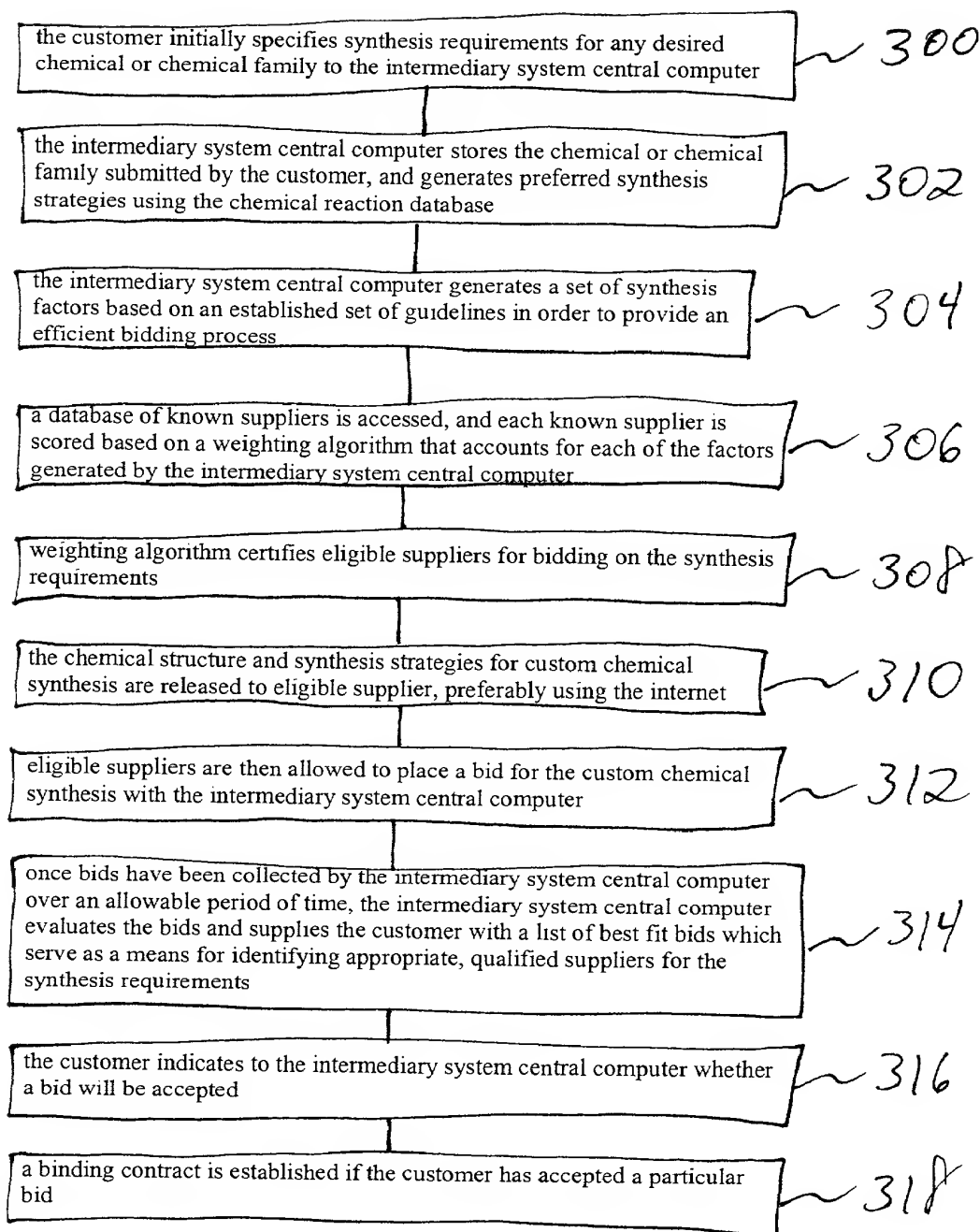


Fig. 5

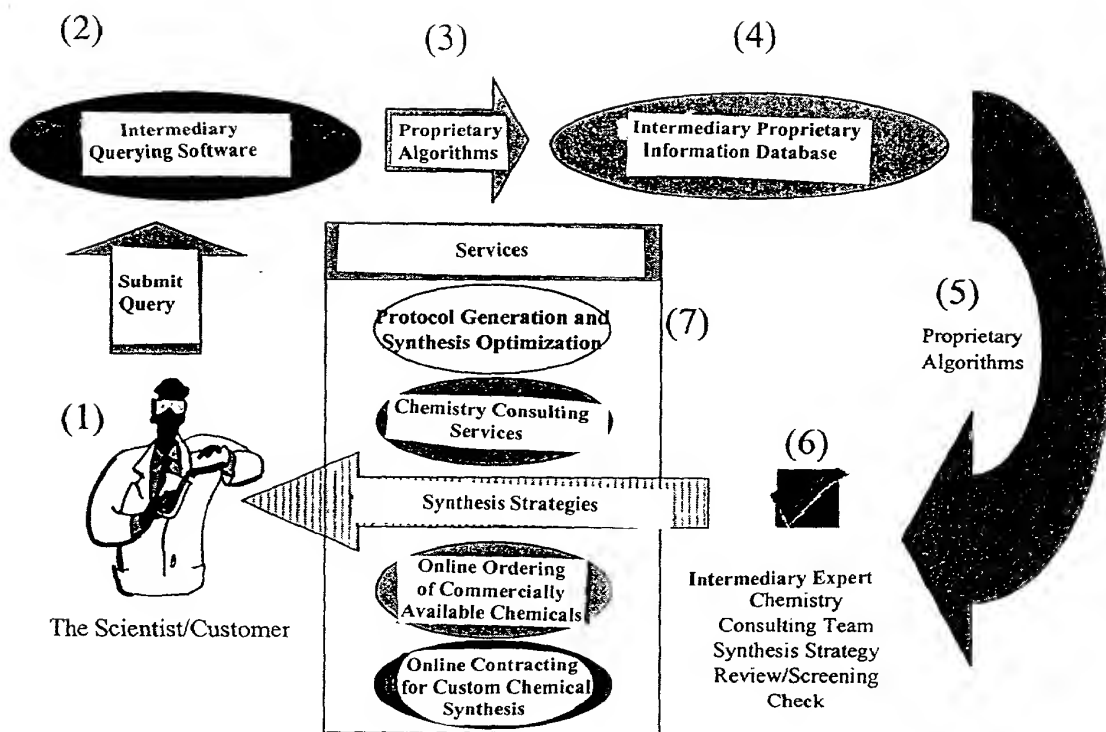
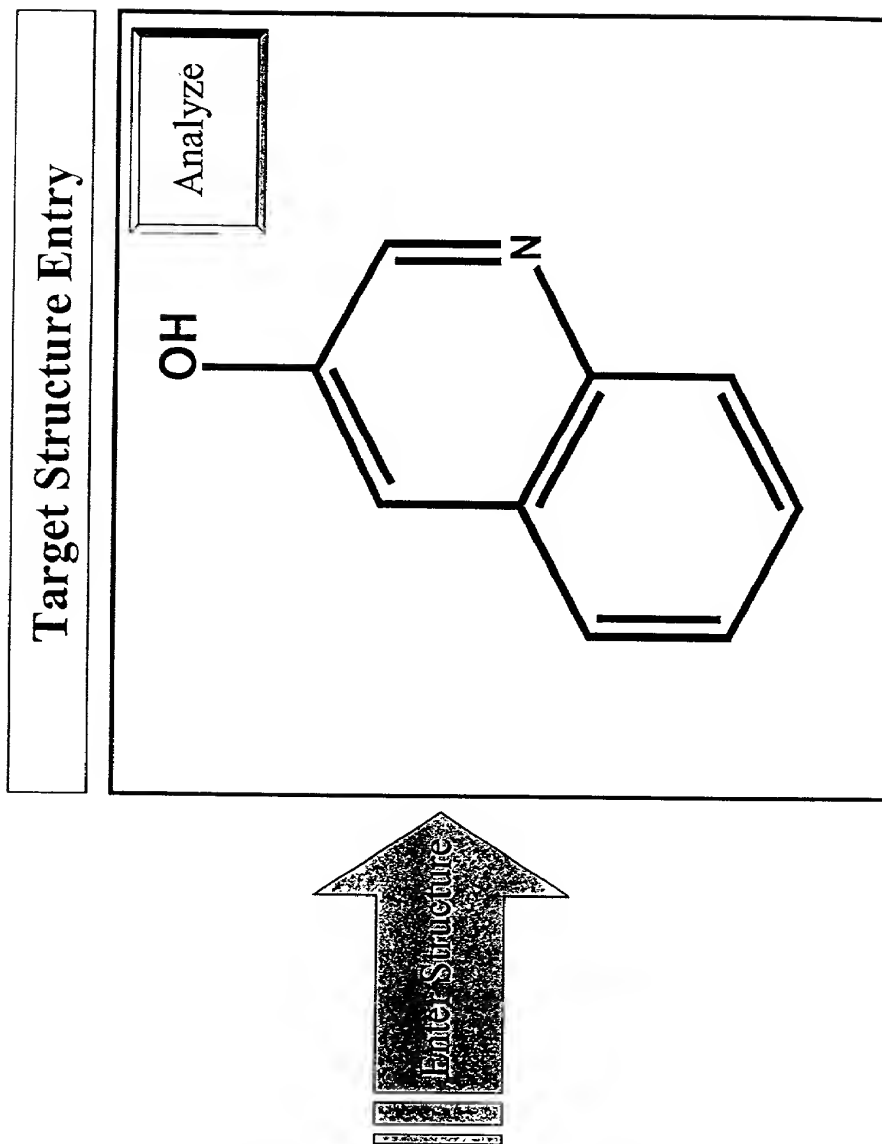


Fig. 6



400

Fig. 7

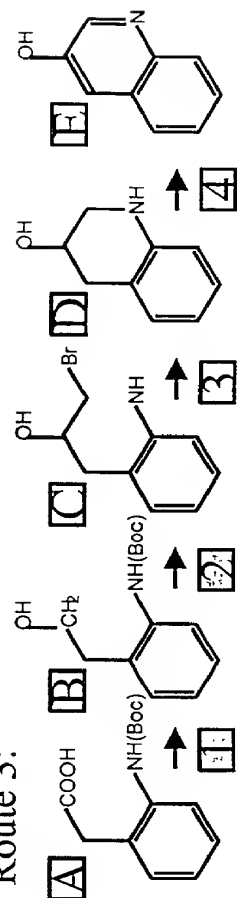
Fig. 8

420

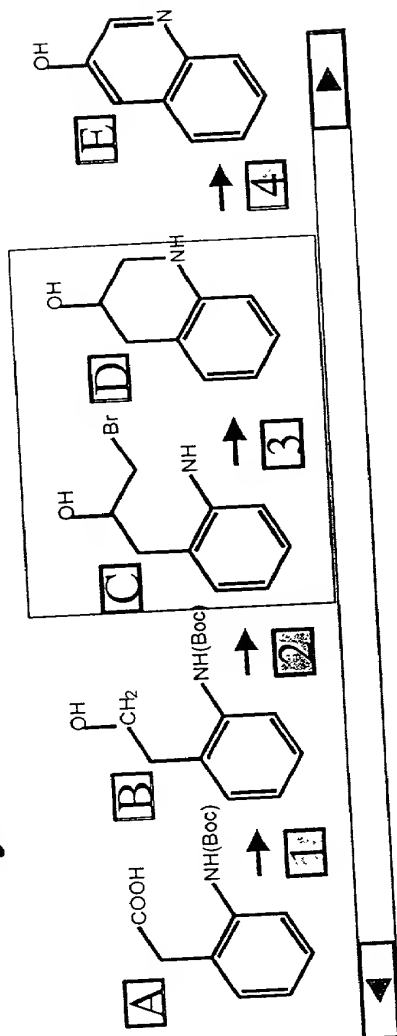
Synthesis Strategies

Routes	Yield %	# of steps to ACD	# of Purification Steps Required	Cost Per mg of product	Add Synthetic Routes to Project
Route 1	86	6	4	\$2,000	<input checked="" type="checkbox"/>
Route 2	75	N/A	N/A	N/A	<input checked="" type="checkbox"/>
Route 3	71	4	3	\$6,434	<input checked="" type="checkbox"/>
Route 4	63	5	2	\$200	<input checked="" type="checkbox"/>
Route 5	44	10	8	\$22,050	<input type="checkbox"/>
Route 6	31	7	6	\$15,427	<input type="checkbox"/>
Route 7	24	5	5	\$155	<input type="checkbox"/>
Route 8	20	6	4	\$4,450	<input type="checkbox"/>
Route 9	17	6	5	\$344	<input type="checkbox"/>
Route 10	9	N/A	N/A	N/A	<input type="checkbox"/>
Route 11	4	6	6	\$36,000	<input type="checkbox"/>

Route 3:



Synthesis Reaction Planner



Amt of Target Compound Desired: XX (g)

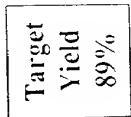
Step	Starting Materials	ID #	Quantity Required	Suggested Supplier	Cost	Place Orders to Suppliers	Request Bids	Inventory location/ Expected arrival date	Scheduled date for completion
[3]	DMF					<input checked="" type="checkbox"/>			
	KOH						<input checked="" type="checkbox"/>	A10233	
	[C]						<input checked="" type="checkbox"/>		
	YYY					<input checked="" type="checkbox"/>			

Fig. 9

440

Fig. 10

460



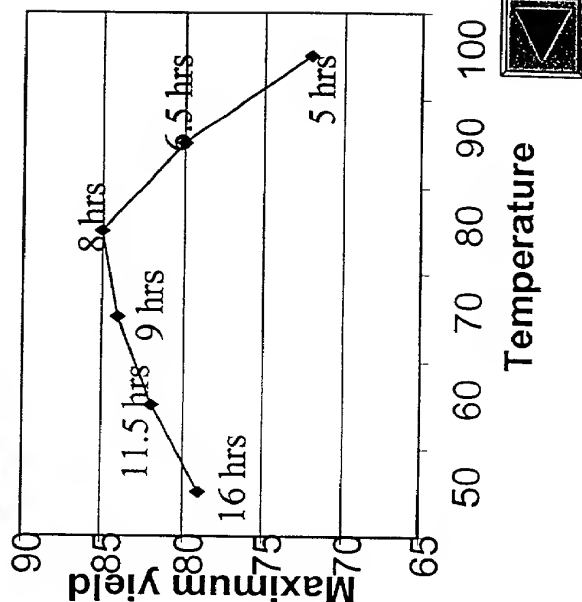
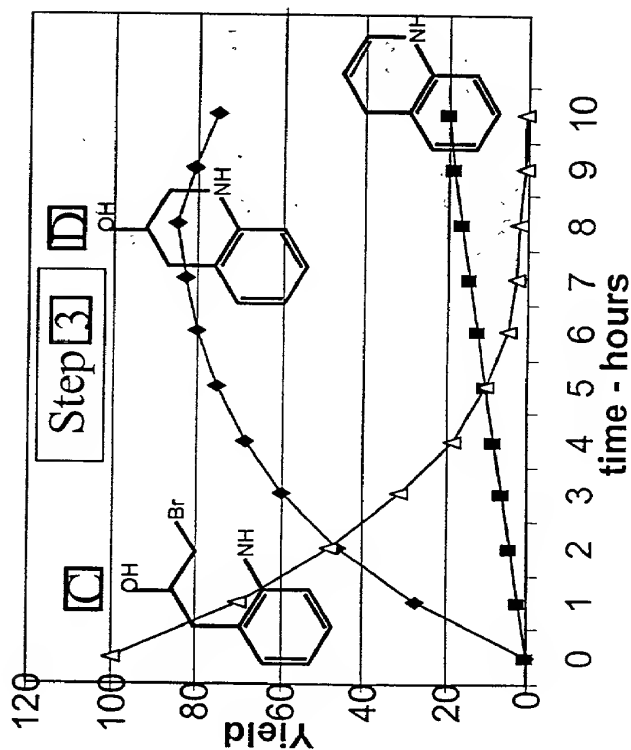
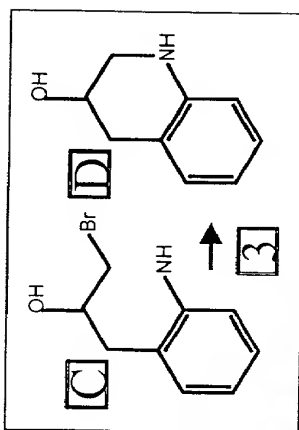
Step	Starting materials in order of addition	Amount (g)	Inventory ID and Location	Solvent	Amount (ml)	Recommended purification steps	Time	Temp.	Scheduled date for completion
3						View Side Products		Optimize	

Fig. 11

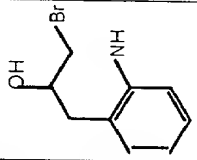

480

Synthesis Reaction Optimization

Optimize the Reaction Time and Temperature for Step [3]	
Temperature	80° C
Time	8 Hrs



Request Bids

Target	Level of Confidentiality Required	Desired Quantity	Cost	Level of Purity	Stereo-chemical Requirements	Suggested Strategies	Request Bids
 	Ultra High Medium Low None	10 g	< \$40,000	~99% ~95% ~90%	None	<div>Edit</div>	<div>Request Preliminary Bids</div> <div>Request Binding Bids</div>

500

Fig. 12